Hexachloropropene

1888-71-7 | DTXSID7062039

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.12e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.76e-01

Confidence level: 5.85e-01

Nearest Neighbors from the Training Set

Image not found
Hexachloropropene
Measured: 6.84e-05
Predicted: 2.12e-04

Image not found
1,2-Dibromo-3-chloropropane
Measured: 4.69e-03
Predicted: 2.20e-03

Image not found
Hexachloro-1,3-butadiene
Measured: 1.23e-05
Predicted: 1.79e-05

Image not found
Pentachloroethane
Measured: 2.37e-03
Predicted: 2.48e-03